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SECURITY CLASSIFICATION OF THIS PAGE

AD-A162 722

(2)

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION: UNCLASSIFIED	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT: Approved for public release; distribution unlimited.
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S): AFOSR-TR- 85-1120
6a. NAME OF PERFORMING ORGANIZATION: State University of New York; 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION: Air Force Office of Scientific Research
6c. ADDRESS (City, State and ZIP Code): Applied Math. & Statistics Dept. Stony Brook, N. Y. 11794	7b. ADDRESS (City, State and ZIP Code): Directorate of Mathematical & Information Sciences, Bolling AFB DC 20332
8a. NAME OF FUNDING/SPONSORING ORGANIZATION: AFOSR; 8b. OFFICE SYMBOL (If applicable): NM	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: AFOSR-84-0383
8c. ADDRESS (City, State and ZIP Code): Bolling AFB DC 20332	10. SOURCE OF FUNDING NOS.: PROGRAM ELEMENT NO. 61102F; PROJECT NO. 2304; TASK NO. A3; WORK UNIT NO.
11. TITLE (Include Security Classification): NUMERICAL METHODS FOR DIFFERENTIAL EQUATIONS	

12. PERSONAL AUTHOR(S): Dr. Reginald P. Tewarson

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Yr., Mo., Day)	15. PAGE COUNT
Annual Report	FROM 30 Sep 84 TO 29 Sep 85		9

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB. GR.	Computer code, variable order, finite difference scheme,

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

During thepast year the investigators have been able to develop a computer code which has turned out to be quite competitive with a well established code. The new approach implements a variable order finite difference scheme which does not require derivatives of the given function and which uses no informaion outside a subinterval to approximate the given system in that subinterval. Three papers have been published as a result of this effort, with the following titles, 'An adaptive boundary value Runge-Kutta solver for first order boundary value problems', 'on the solution of sparse non-linear ewuations and some applications' adn 'A quasi-Newton method with sparse triple factorization'. Four additional papers are in press.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT: UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS ☐	21. ABSTRACT SECURITY CLASSIFICATION: UNCLASSIFIED
22a. NAME OF RESPONSIBLE INDIVIDUAL: JOHN P, THOMAS, Jr., Capt, USAF	22b. TELEPHONE NUMBER (Include Area Code): (202) 767- 5026; 22c. OFFICE SYMBOL: NM

DD FORM 1473, 83 APR — EDITION OF 1 JAN 73 IS OBSOLETE.

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SECURITY CLASSIFICATION OF THIS PAGE

AFOSR-TR- 85-1120

ANNUAL TECHNICAL REPORT

September 30, 1984 to September 29, 1985

Grant Number: AFOSR-84-0383

Title: Numerical Methods for Differential Equations

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Annual Report

Grant No: AFOSR-84-0383

SUMMARY

The overall long term goals of this research project are: to develop efficient computational algorithms and new, readily transportable, competitive general purpose computer codes for the numerical solution of two point boundary value differential equations; to use these techniques to develop adaptive codes for stiff and non-stiff initial value problems and the method of lines for the solution of partial differential equations; to test the codes on problems arising in diverse application areas, e.g., Physics, Chemistry, Fluid Mechanics, Combustion and Biomathematics.

The short term goal is to develop and implement variable order finite difference schemes which do not require derivatives of the given function and use no information outside a subinterval to approximate the given system of differential equations in that subinterval and use a variation of deferred correction for the solution of the corresponding non-linear algebraic equations.

During the past year the investigators have been able to develop a computer code which, on the basis of some preliminary experiments, has turned out to be quite competitive with a well established code. Extensive test are planned during the coming year. The algorithmic development phase of the research has led

to several useful results. An eighth order method, which has second, fourth and sixth order methods embedded in it has been developed. The method possesses some of the best features of implicit Runge-Kutta and Gap schemes. A multiderivative generalization of the above schemes has also been realized. A sparse factorization for quasi-Newton type methods has been obtained. Algorithms for solving combined systems of linear and non-linear algebraic equations and matrix splitting have also been developed.

Some of our results have been used for the computer simulation of kidney function at the Cornell Medical School in a collaborative research in which the Principal Investigator is involved.

REPORT

Finite difference methods which combine features of both Runge-Kutta processes and Gap schemes have been developed [1]. These methods are suitable for use in adaptive codes for the solution of first order differential equations with two-point boundary conditions. Success has been achieved in finding the order conditions for these methods and also some techniques that can be used to reduce the order number. An eighth order method which has second, fourth and sixth order methods embedded in it has been developed. This eighth order method as well as embedded methods are A-stable. A technique has been proposed which exploits the natural embedding of methods for the estimation of the error in the numerical solution. This natural embedding of the methods is also utilized to estimate the local truncation error. In turn, these truncation error estimates are used to generate asymptotically equidistributing meshes using adaptive mesh placement procedures. A quasi-Newton method is described in this paper for solving discretized systems arising from the use of proposed methods. It has been possible to developed a preliminary general purpose adaptive code based on these methods.

A general description of sparsity based algorithms that use structural information in handling the model equations is given in [2]. The primary focus is on splitting of equations and variables into two subsets: one large but relatively easy to solve, called the non-basic subset, and the other small but difficult to handle, called the basic subset. The non-basic subset is then solved more often than the difficult basic set. The computer storage is that required by the basic set. Applications in flow networks and energy-economy models are briefly described.

A new quasi-Newton method for sparse matrices arising in various application areas is presented in [3]. In this work sparse triple factorization is used to develop a rank two update.

In [4], multi-derivative generalizations of the processes given in [1] are considered. These use fewer derivatives to yield results analogous to those for Gap schemes. Obviously, these processes instead of Gap schemes should be utilized if the higher order analytic derivatives are not readily available.

An efficient method for handling systems with linear and non-linear subsystems is given in [5]. In this method iterations are needed only for the solution of non-linear subsystems.

Cubic and quintic splines have been utilized in some of the methods for solving differential equations developed by the investigators and others in the past . One of the crucial steps in these techniques involves the solution of band systems. A very efficient general purpose scheme for handling such band systems [6] has been developed. This scheme is also very useful for block banded systems arising in a variety of applications.

A method of order eight that uses cubic splines on quintic splines for solving differential equations is described in [7].

A class of processes [8] have been found for solving second order boundary value problems of the form $y'' = f(x,y)$, $y(a)=A$, $y(b)=B$. These do not require derivatives of f, and result in nonlinear equations with blocked tridiagonal Jacobians. Specialized techniques have been developed to derive the necessary formulas. The computation of the Jacobians for the discretized systems arising from the use of these formulas is expensive. This makes the ordinary Newton iterations impractical. This paper contains various techniques for approximating and splitting the Jacobians. These techniques are computationally inexpensive and lead to excellent convergence.

The Principal Investigator has given invited papers based on some of the research resulting from this grant at two international conferences [9,10]. One of the problems in the solution of large systems of non-linear algebraic equations arising in the numerical solution of differential equations is to be able to choose the starting approximate solution in the domain of attraction of the desired solution. Continuation type methods are used to enlarge this domain of attraction. An algorithm (based on Moore-Penrose generalized inverse) to handle the turning points in continuation methods has been developed.

PUBLICATIONS

(a) Published papers:

1. S. Gupta, An adaptive boundary value Runge-Kutta solver for first order boundary value problems, SIAM J. Numer Anal., 22 (1985), pp. 114-126.
2. R.P. Tewarson, On the solution of sparse non-linear equations and some applications, in Sparsity and Applications, D. J. Evans (Ed), Cambridge University Press, 1984, 137-152.
3. D. Q. Chen and R. P. Tewarson, A quasi-Newton method with sparse triple factorization, Computing 33 (1984), 315-329.

(b) Papers in Press:

4. S. Gupta, Multi-derivative Runge-Kutta Processes for two-point boundary value problems, BIT 25(1985), 233-241.

5. R. P. Tewarson and D. Q. Chen, A method for solving Algebraic Systems consisting of linear and nonlinear equations, Int. J. Num. Meth. in Engr. (1984), to appear.

6. D. Q. Chen and R. P. Tewarson, Use of incomplete decomposition of the coefficient matrix in solving linear equations, Int. J. Num. Meth. in Engr. (1985), to appear.

7. R. P. Tewarson and Y. Zhang, Solution of two-point boundary value problems using splines, Int. J. Num. Meth. in Engr. (1985), to appear.

(c) Papers Submitted for Publication:

8. [illegible]. Gupta, Numerical methods and matrix splitting for higher order two-point boundary value problems, Proc. of International Conference on Future Trends in Computing, Grenoble, France, 1985, (to appear).

(d) Invited Talks:

9. R. P. Tewarson, Models of flow networks, Fifth International Conference on Mathematical Modeling, July 29-31, 1985, Berkeley, Calif.

10. R. P. Tewarson, Use of mathematical models in the computer simulation of flow networks, International Symposium

on Mathematical Modeling of Ecological, Environmental and Biological Systems, August 27-30, Indian Institute of Technology, Kanpur, India. To be published as Conference Proceedings.

(e) Contributed Talks:

11. S. Gupta, Numerical methods and matrix splitting for boundary value problems, SIAM Conf., Raleigh, N. C., April 29 - May 3, 1985.

12. S. Gupta, Numerical methods for higher order boundary value problems, Grenoble, France, Dec. 2-6, 1985.